

# Hestenes Method for Symmetric Indefinite Systems in Interior-Point Method \*

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## Abstract

This paper deals with the analysis and the solution of the Karush–Kuhn–Tucker (KKT) system that arises at each iteration of an Interior–Point (IP) method for minimizing a nonlinear function subject to equality and inequality constraints.

This system is generally large and sparse and it can be reduced so that the coefficient matrix is still sparse, symmetric and indefinite, with size equal to the number of the primal variables and of the equality constraints.

Instead of transforming this reduced system to a quasidefinite form by regularization techniques used in available codes on IP methods, under standard assumptions on the nonlinear problem, the system can be viewed as the optimality Lagrange conditions for a linear equality constrained quadratic programming problem, so that Hestenes multipliers' method can be applied.

Numerical experiments on elliptic control problems with boundary and distributed control show the effectiveness of Hestenes scheme as inner solver for IP methods.

## Sunto

Questo lavoro riguarda la risoluzione del sistema di Karush–Kuhn–Tucker (KKT) che occorre risolvere ad ogni iterazione dei metodi del Punto Interno (IP) per minimizzare funzioni non lineari soggette a vincoli di uguaglianza e di disuguaglianza. Il sistema è generalmente sparso e di grandi dimensioni e può essere ridotto in modo che la matrice dei coefficienti sia ancora sparsa, simmetrica e indefinita di ordine uguale al numero delle variabili primali e dei vincoli di uguaglianza.

Invece di trasformare il sistema ridotto ad una forma quasi definita mediante le tecniche di regolarizzazione presenti nei codici per i metodi IP, sotto le classiche ipotesi sul problema non lineare, si può osservare che il sistema esprime le condizioni di ottimalità di Lagrange per un problema di programmazione quadratica con vincoli lineari di uguaglianza; in tal caso, è possibile applicare il metodo dei moltiplicatori di Hestenes.

Esperimenti numerici su problemi ellittici di controllo ottimo con controllo definito sul contorno o distribuito sul dominio, mostrano l'efficienza dello schema di Hestenes come risolutore interno per i metodi IP.

**Keywords:** Indefinite symmetric reduced KKT system, Newton Inexact Interior–Point method, large scale nonlinear programming problems, Hestenes multipliers' method, elliptic control problems.

**AMS subject classification:** 65K05, 90C26, 90C51.

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# 1 The symmetric indefinite systems in Interior–Point methods

This paper is concerned with the numerical solution of large and sparse nonlinear nonconvex programming problems by a Newton Interior–Point (IP) method. We consider general problems of the form

$$\begin{aligned} \min & f(\mathbf{x}) \\ & \mathbf{g}_1(\mathbf{x}) = 0 \\ & \mathbf{g}_2(\mathbf{x}) \geq 0 \\ & \mathbf{x}_{\mathcal{L}} \geq \mathbf{l} \\ & \mathbf{x}_{\mathcal{U}} \leq \mathbf{u} \end{aligned} \quad (1)$$

where  $\mathbf{x} \in \mathbb{R}^n$ ,  $f(\mathbf{x}) : \mathbb{R}^n \rightarrow \mathbb{R}$ ,  $\mathbf{g}_1(\mathbf{x}) : \mathbb{R}^n \rightarrow \mathbb{R}^{n_{eq}}$ ,  $\mathbf{g}_2(\mathbf{x}) : \mathbb{R}^n \rightarrow \mathbb{R}^m$ ,  $\mathbf{l} \in \mathbb{R}^{n_l}$ ,  $\mathbf{u} \in \mathbb{R}^{n_u}$ ,  $\mathcal{L}$  and  $\mathcal{U}$  are subsets of the index set  $\{1, \dots, n\}$  and  $f(\mathbf{x})$ ,  $\mathbf{g}_1(\mathbf{x})$ ,  $\mathbf{g}_2(\mathbf{x})$  are twice continuously differentiable.

By introducing slack variables  $\tilde{\mathbf{s}} \in \mathbb{R}^{m+n_l+n_u}$  for the inequality and box constraints, the Karush–Kuhn–Tucker (KKT) optimality conditions for problem (1) can be expressed as a nonlinear system

$$\begin{aligned} \mathbf{H}(\mathbf{v}) &= 0 \\ \tilde{\mathbf{s}} &\geq 0; \quad \tilde{\mathbf{w}} \geq 0 \end{aligned}$$

where  $\mathbf{v} = (\mathbf{x}^t, \boldsymbol{\lambda}_1^t, \tilde{\mathbf{w}}^t, \tilde{\mathbf{s}}^t)^t$ ,  $\boldsymbol{\lambda}_1$  is the vector of multipliers corresponding to the equality constraints,  $\tilde{\mathbf{w}} \in \mathbb{R}^{m+n_l+n_u}$  is the vector of multipliers corresponding to the inequality and box constraints.

In the framework of IP methods, instead of solving the previous nonlinear system, we have to solve the following perturbed KKT conditions

$$\begin{aligned} \mathbf{H}(\mathbf{v}) &= \rho_k \tilde{\mathbf{e}} \\ \tilde{\mathbf{s}} &> 0; \quad \tilde{\mathbf{w}} > 0 \end{aligned} \quad (2)$$

where  $\rho_k$  is a positive perturbation parameter.

A crucial issue for an efficient implementation of the class of IP methods is the solution of the following linear system

$$\mathbf{H}'(\mathbf{v}^{(k)}) \Delta \mathbf{v} = -\mathbf{H}(\mathbf{v}^{(k)}) + \rho_k \tilde{\mathbf{e}} \quad (3)$$

that determines at each  $k$ -th iteration the descent direction  $\Delta \mathbf{v}^{(k)}$  used to update the current iterate:

$$\mathbf{v}^{(k+1)} = \mathbf{v}^{(k)} + \alpha_k \Delta \mathbf{v}^{(k)} \quad (4)$$

where  $\tilde{\mathbf{e}} = (\mathbf{0}_{n+n_{eq}}^t, \mathbf{1}_{m+n_l+n_u}^t)^t$ .

The formulae (3) and (4) represent the damped Newton iteration for determining the numerical solution of the nonlinear system (2).

By using an elimination technique (see [3]), the linear system (3) can be reduced to an indefinite symmetric system, known as KKT reduced system, having the following form

$$\begin{pmatrix} -A & B \\ B^t & 0 \end{pmatrix} \begin{pmatrix} \Delta \mathbf{x} \\ \Delta \boldsymbol{\lambda}_1 \end{pmatrix} = \begin{pmatrix} \mathbf{c} \\ \mathbf{q} \end{pmatrix} \quad (5)$$

where  $A \in \mathbb{R}^{n \times n}$ ,  $B^t \in \mathbb{R}^{neq \times n}$  and, for simplicity, we omit the index iteration  $k$ . The matrix  $A$  is the sum of three matrices: the hessian of the lagrangian function of the problem (1), a positive semidefinite matrix  $\nabla \mathbf{g}_2(\mathbf{x}) T \nabla \mathbf{g}_2(\mathbf{x})^t$  (where  $T$  is a positive diagonal matrix) and a diagonal nonnegative matrix deriving from the slack variables and the vectors of multipliers related to the box constraints. The matrix  $B^t$  is equal to  $\nabla \mathbf{g}_1(\mathbf{x})$ . A special version of the system (5) arises when the equality constraints are formulated as inequalities (see LOQO code [17])

$$0 \leq \mathbf{g}_1(\mathbf{x}) \leq 0$$

and they are transcribed in the form

$$\begin{aligned} \mathbf{g}_1(\mathbf{x}) - \mathbf{s}_1 &= 0 \\ \mathbf{s}_1 + \mathbf{p}_1 &= 0 \\ \mathbf{s}_1 &\geq 0; \quad \mathbf{p}_1 \geq 0 \end{aligned}$$

The final system has the form

$$\begin{pmatrix} -\tilde{A} & \tilde{B} \\ \tilde{B}^t & \tilde{E} \end{pmatrix} \begin{pmatrix} \Delta \mathbf{x} \\ \Delta \boldsymbol{\lambda} \end{pmatrix} = \begin{pmatrix} \tilde{\mathbf{c}} \\ \tilde{\mathbf{q}} \end{pmatrix} \quad (6)$$

where  $\tilde{E} \in \mathbb{R}^{(m+neq) \times (m+neq)}$  is a diagonal matrix with strictly positive entries representing the contribution of the slack variables and the vectors of multipliers corresponding to constraints  $\mathbf{g}_1(\mathbf{x}) = 0$  and  $\mathbf{g}_2(\mathbf{x}) \geq 0$ ;  $\tilde{B}^t = (\nabla \mathbf{g}_1(\mathbf{x}), \nabla \mathbf{g}_2(\mathbf{x}))^t$  and  $\tilde{A}$  is the sum of the hessian of the lagrangian function of the problem (1) and of a diagonal nonnegative matrix deriving from the slack variables and the vectors of multipliers related to the box constraints.

For the well definiteness of the IP method, it is required that at each iteration the systems (5) and (6) are nonsingular. Furthermore, in many real life applications, the matrices  $A$  or  $\tilde{A}$  are large and sparse and they can be also singular.

In the framework of the direct methods ([9], [8]), the solution of the systems (5) or (6) is obtained by the sparse symmetry preserving Bunch–Parlett triangular factorization  $LDL^t$  ([4], [5], [2]), where  $L$  is a triangular matrix and  $D$  is a block diagonal matrix with  $1 \times 1$  and  $2 \times 2$  pivots. This approach, like any other factorization that combines dynamic reordering for sparsity preserving and pivoting technique for numerical stability, can be very expensive.

Another strategy, used by more recent IP solvers, is to transform the symmetric systems (5) and (6) to a *quasidefinite* form [18]. A symmetric matrix is quasidefinite if it has the form

$$\begin{pmatrix} -F & S \\ S^t & E \end{pmatrix} \quad (7)$$

where  $F$  and  $E$  are symmetric positive definite square matrices. For any symmetric permutation  $P$  (also for  $P = I$ ), a quasidefinite matrix is *strongly factorizable*, that is, it can be factorized in a Cholesky–like form  $\tilde{L}\tilde{D}\tilde{L}^t$ , where  $\tilde{L}$  is a triangular matrix and  $\tilde{D}$  is a diagonal matrix with negative entries in the rows corresponding to  $F$  block and positive entries in the rows corresponding to  $E$  block. This factorization enables us to perform eventually an a–priori sparsity preserving reordering of the matrix that takes into account

only its structure. See, for example, the *priority minimum-degree technique* used in the code LOQO and described in [18] that is performed in an analysis phase, before to begin the IP iterations. In this technique, the columns of the matrix (7) are separated in two groups: the columns corresponding to the matrix  $F$  form the primal group and those corresponding to the matrix  $E$  form the dual group. If the pivots are initially chosen in the primal group, a minimum degree reordering technique is used within each group and the matrix that must be factorized for the second group is a symmetric permutation of  $N_P = S^t F^{-1} S + E$  (primal method). When the pivots are initially chosen in the dual group, since  $E$  is equal to  $\tilde{E}$  of (6) that is a positive diagonal matrix, no reordering is performed in this group; a minimum degree reordering is performed only on the matrix  $N_D = F + S E^{-1} S^t$  (dual method). For linear and convex quadratic programming (where  $F = \tilde{A}$  is positive definite), the LOQO code chooses between primal and dual method to maximize sparsity in the factorization, taking into account of a heuristic which estimates the fill-in produced by the two techniques. For nonlinear programming, where the indefinite matrix  $\tilde{A}$  can be singular, the dual method is always chosen since the semipositive definite term  $\tilde{B} E^{-1} \tilde{B}^t$  can make the matrix  $\tilde{A} + \tilde{B} \tilde{E}^{-1} \tilde{B}^t$  positive definite.

In order to transform the matrices of (5) and of (6) to a quasidefinite form, it is possible to use a *regularization* technique. In the case of system (5) a convenient diagonal matrix is added to the whole coefficient matrix:

$$\begin{pmatrix} -A & B \\ B^t & 0 \end{pmatrix} + \begin{pmatrix} -R_P & 0 \\ 0 & R_D \end{pmatrix} \quad (8)$$

where the diagonal nonnegative matrices  $R_P$  and  $R_D$  are called primal regularization matrix and dual regularization matrix respectively. In the case of system (6), the regularization is obtained by adding only to the block  $\tilde{A}$  a primal regularization diagonal matrix. This last approach is followed by Vanderbei [17]. In particular, when the matrix  $N_D$  is not positive definite, that is some diagonal pivot is zero or negative, the matrix  $\tilde{A}$  is perturbed by computing  $\tilde{A} + \rho I$ , where  $\rho$  is a positive parameter with an initial heuristic value. If the initial value of  $\rho$  is too small, this value is doubled until a Cholesky-like factorization is obtained. If, on the other hand, the initial value of  $\rho$  is too large, successive halving of the parameter are performed until we find the minimum perturbation value that permits the Cholesky-like factorization.

The regularization technique (8) is used in [11], where  $R_P = \gamma^2 I$  and  $R_D = \delta^2 I$  are a priori fixed. On the contrary, in [1] the matrices  $R_P$  and  $R_D$  are *dynamically* computed; in the code implementing the Cholesky-like factorization, when a critical pivot is reached, this is perturbed by a small quantity. In practical, when a pivot  $d_{ii}$  has a wrong sign and/or  $|d_{ii}| < \epsilon \max_{i=1,n} |a_{ii}|$ , where  $\epsilon$  is the machine precision and  $a_{ii}$  are the diagonal entries of  $A$ , the corresponding  $i$ -th element of the regularization matrix  $R_P$  or  $R_D$  is nonnull.

In this work, we propose a different approach that avoids modifications of the matrices of the problem. Under suitable conditions, the reduced KKT system (5) can be viewed as the Lagrange necessary conditions for the minimum point of a linear equality constrained quadratic programming problem. Consequently, it can be efficiently solved by the iterative Hestenes multipliers' scheme. In this way, the solution of the KKT indefinite system is led to the solution of a sequence of smaller symmetric positive definite systems that can be solved by efficient sparse Cholesky codes. Since the Hestenes scheme is an iterative solver, it is convenient to use an adaptive stopping rule for this inner solver, so that unnecessary

inner iterations are avoided when we are far from the solution. A suitable termination criterium is devised in the Newton Inexact IP method described in [6] (see also [7]) where, under hypotheses very similar to those of a Newton IP method, the global convergence of the scheme is proved.

In the last section, numerical experiments show that, generally, one or two iterations of the Hestenes scheme are sufficient to satisfy the inner adaptive stopping rule. As consequence, since the Newton Inexact IP method preserves the good behaviour of the classical Newton IP methods, the proposed approach appears very promising for an efficient solution of a nonlinear programming problem.

## 2 The Hestenes multipliers' scheme for the solution of the reduced KKT system

Let  $B^t$  be a full row-rank matrix. In order to analyze the features of the system (5), it is necessary to introduce the  $n \times (n - neq)$  matrix  $Z$  such that  $B^t Z = 0$  and  $Z^t Z = I$ . Then the columns of  $Z$  form an orthonormal basis of  $\mathcal{N}(B^t)$ , the null space of  $B^t$ . The following theorem enables us to state, in terms of  $Z$ , the necessary and sufficient conditions for the nonsingularity of the matrix in (5).

**Theorem 2.1** ([10]) Let  $k_+, k_-$  and  $k_0$  be the number of positive, negative and zero eigenvalues of the matrix  $M = \begin{pmatrix} A & -B \\ -B^t & 0 \end{pmatrix}$ , where  $A \in \mathbb{R}^{n \times n}$ ,  $B^t \in \mathbb{R}^{neq \times n}$  of full row-rank, and let  $l_+, l_-$  and  $l_0$  be the number of positive, negative and zero eigenvalues of the matrix  $Z^t A Z$ . Then  $k_- = l_- + neq$ ,  $k_+ = l_+ + neq$  and  $k_0 = l_0$ .

As consequence,  $M$  is a nonsingular matrix if and only if  $Z^t A Z$  is a nonsingular matrix. In particular, a sufficient condition for the nonsingularity of  $M$  is that the matrix  $Z^t A Z$  is positive definite (see also [14, p. 424]). Then, to guarantee the well definiteness of the Newton Inexact Interior-Point method, we assume that this condition holds at each iteration of the scheme.

This condition holds if the hessian matrix of the lagrangian function of the problem (1) is positive definite on the null space of  $B^t$ . Note that this assumption is also the one required for the local SQP method ([16, p. 531]).

Setting  $\mathbf{y}_1 = \Delta \mathbf{x}$  and  $\mathbf{y}_2 = \Delta \boldsymbol{\lambda}_1$ , the system (5), can be viewed as the Lagrange necessary conditions for the minimum point of the following quadratic problem

$$\begin{aligned} \min \quad & \frac{1}{2} \mathbf{y}_1^t A \mathbf{y}_1 + \mathbf{c}^t \mathbf{y}_1 \\ & B^t \mathbf{y}_1 - \mathbf{q} = 0 \end{aligned}$$

This quadratic problem can be solved efficiently by Hestenes' multipliers scheme ([12]), that consists in updating the dual variable by the rule

$$\mathbf{y}_2^{(j+1)} = \mathbf{y}_2^{(j)} + \chi (B^t \mathbf{y}_1^{(j)} - \mathbf{q})$$

where  $\chi$  is a positive parameter (penalty parameter) and  $\mathbf{y}_1^{(j)}$  minimize the augmented lagrangian function of the quadratic problem

$$\mathcal{L}_\chi(\mathbf{y}_1, \mathbf{y}_2) = \frac{1}{2} \mathbf{y}_1^t A \mathbf{y}_1 + \mathbf{y}_1^t \mathbf{c} + \mathbf{y}_2^t (B^t \mathbf{y}_1 - \mathbf{q}) + \frac{\chi}{2} (B^t \mathbf{y}_1 - \mathbf{q})^t (B^t \mathbf{y}_1 - \mathbf{q})$$

This means that  $\mathbf{y}_1^{(j)}$  is the solution of the linear system of order  $n$

$$(A + \chi BB^t)\mathbf{y}_1 = -B\mathbf{y}_2^{(j)} - \mathbf{c} + \chi B\mathbf{q} \quad (9)$$

Note that, since  $B^t$  has full row-rank, the null space of  $BB^t$  is equal to the null space of  $B^t$ , then the matrix  $A$  is positive definite on the null space of  $BB^t$ . Then, it is immediate the following theorem.

**Theorem 2.2** ([14, p. 408]) If  $Z^tAZ$  is a positive definite matrix and  $B^t$  has a full row-rank, there exists a positive value  $\chi^*$  such that for all  $\chi > \chi^*$ , the matrix  $A + \chi BB^t$  is positive definite.

This result enables us to solve the system (9) by applying a Cholesky factorization. The computational complexity due to matrix-matrix products  $\nabla \mathbf{g}_2(\mathbf{x})^T \nabla \mathbf{g}_2(\mathbf{x})$  (to compute the matrix  $A$ ) and  $BB^t$  are unavoidable. Indeed, in a Cholesky-like factorization, the computation of the matrix  $N_D$  or a similar matrix is also required. Then, in order to save computing time at each iteration, it is convenient to perform an a priori symbolic computation that devises the nonzero entries of the matrix-matrix products and the indices of the nonzero elements that form these entries; then an a priori minimum degree reordering enables us to preserve the sparsity of the matrices (see [13]).

In order to choose the parameter  $\chi$ , we observe that, for all  $\mathbf{x} \neq 0$ , we must have  $\mathbf{x}^t(A + \chi BB^t)\mathbf{x} > 0$ . When  $B^t\mathbf{x} = 0$ , we have  $\mathbf{x}^tA\mathbf{x} > 0$ . If  $B^t\mathbf{x} \neq 0$ ,  $\mathbf{x}^tBB^t\mathbf{x} > 0$ . Then, it follows that

$$\chi > \max(0, \max_{\mathbf{x} \notin N(B^t)} \frac{-\mathbf{x}^tA\mathbf{x}}{\mathbf{x}^tBB^t\mathbf{x}})$$

Since  $\|A\| \geq -\mathbf{x}^tA\mathbf{x}/\|\mathbf{x}\|^2$  for any natural norm and also for the Frobenius norm  $\|\cdot\|_F$ , and  $\mathbf{x}^tBB^t\mathbf{x}/\|\mathbf{x}\|^2 \geq \tau_{min}$ , where  $\tau_{min}$  is the minimum nonzero eigenvalue of  $BB^t$  or of  $B^tB$ , we can choose as  $\chi$  the following value:

$$\chi > \frac{\|A\|_F}{\tau_{min}}$$

To approximate  $\tau_{min}$  we can use the minimum diagonal entry  $t_{min}$  of the matrix  $B^tB$ . Furthermore in order to avoid that the value of  $\chi$  is too small (the matrix is not positive definite) or too large (too ill-conditioned system), it is convenient to use safeguards. In the numerical experiments of the next section, the following value of  $\chi$  produced good results:

$$\chi = \max(\min(10^7, \frac{\max\{\|A\|_F, 1\}}{\min\{t_{min}, 1\}}), 10^8) \quad (10)$$

### 3 Numerical Results

In order to evaluate the effectiveness of Hestenes solver for the indefinite system that arises at each step of the Newton Interior-Point method, numerical experiments on two nonlinear programming problems, arising from discretization of elliptic control problems ([15]), have been carried out on Compaq XP1000 workstation with Alpha 21264 ev6 processor 466 Mhz and 784 Mb of RAM.

The first test problem is the following boundary control problem:

$$\min_{y,u} \frac{1}{2} \int_{\Omega_0} (y(x_1, x_2) - 1)^2 dx_1 dx_2 + \frac{\alpha}{2} \int_{\Gamma_2} u(x_1, x_2)^2 dx_1 dx_2 \quad (11)$$

subject to the state equation, Neumann and Dirichlet boundary conditions and control and state inequality constraints

$$\begin{aligned} -\Delta y(x_1, x_2) &= 0 && \text{in } \Omega \\ \partial_\nu y(x_1, x_2) &= 0 && \text{for } x_2 = 0 \quad 0 \leq x_1 \leq 1 \\ \partial_\nu y(x_1, x_2) &= y(x_1, x_2) - 5 && \text{for } x_1 \in (0, 1) \quad 0 \leq x_2 \leq 1 \\ y(x_1, x_2) &= u(x_1, x_2) && \text{for } x_2 = 1 \quad 0 \leq x_1 \leq 1 \\ y(x_1, x_2) &\leq 3.15 && \text{in } \Omega_0 \\ y(x_1, x_2) &\leq 10 && \text{in } \Omega \setminus \Omega_0 \\ 0 \leq u(x_1, x_2) &\leq 10 && \text{for } x_2 = 1 \quad 0 \leq x_1 \leq 1 \end{aligned} \quad (12)$$

where  $\Omega = [0, 1] \times [0, 1]$ ,  $\Omega_0 = [0.25, 0.75] \times [0.25, 0.75]$ ,  $\Gamma$  is the boundary of  $\Omega$  and  $\Gamma_2 = \{(x_1, 1) : 0 \leq x_1 \leq 1\}$ . This problem can be transcribed as a linear constrained quadratic programming problem, by discretizing the objective functional with the rectangular rule and the dynamical system with the five-point formula on a uniform two dimensional mesh of  $(N_h + 1) \times (N_h + 1)$  points. Figures 1 and 2 show the patterns, for  $N_h = 5$ , of the symmetric positive semidefinite hessian matrix and of the matrix  $B^t$  of the constraints respectively.

The second test problem is the following distributed control problem:

$$\min_{y,u} \int_{\Omega} (Mu(x_1, x_2)^2 - Ku(x_1, x_2)y(x_1, x_2)) dx_1 dx_2 \quad (13)$$

subject to the elliptic state equation, homogeneous Neumann boundary conditions and control and state inequality constraints

$$\begin{aligned} -\Delta y(x_1, x_2) &= y(x_1, x_2)(a(x_1, x_2) - u(x_1, x_2) - by(x_1, x_2)) && \text{in } \Omega \\ \partial_\nu y(x_1, x_2) &= 0 && \text{in } \Gamma \\ u_1 \leq u(x_1, x_2) &\leq u_2; \quad y(x_1, x_2) \leq \psi(x_1, x_2) && \text{in } \Omega \end{aligned} \quad (14)$$

where  $\Omega$  is the unit square and  $\Gamma$  its boundary.

By using the same discretization techniques of the previous problem, this problem can be formulated as a nonlinear program with quadratic objective function and nonlinear constraints (see the patterns of the hessian matrix and of the jacobian matrix of the equality constraints in figures 3 and 4 for  $N_h = 5$  and  $M \neq 0$ ). In (14),  $a(x_1, x_2) = 7 + 4\sin(2\pi x_1 x_2)$  and  $b = 1$ .

In figures 1–4, “nz” denotes the number of the nonzero elements of the displayed matrices. Furthermore, Table 1 shows the values of the parameters for the two test problems. In all test problems, both the control and the state become active.

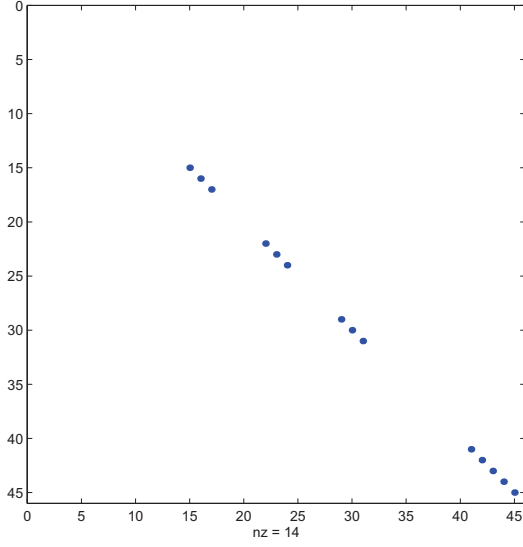


Figure 1

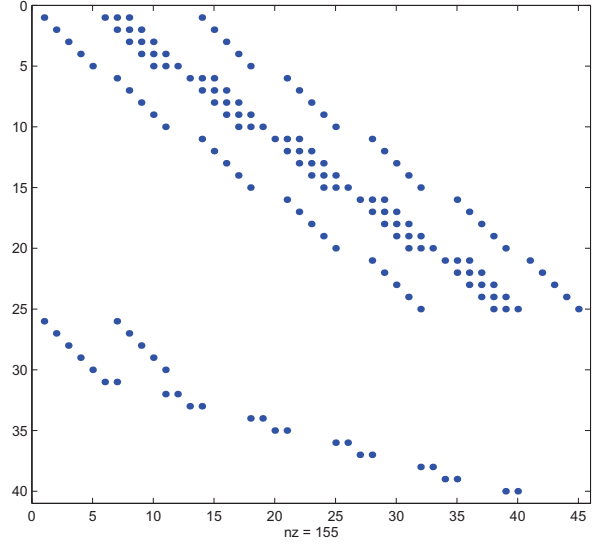


Figure 2

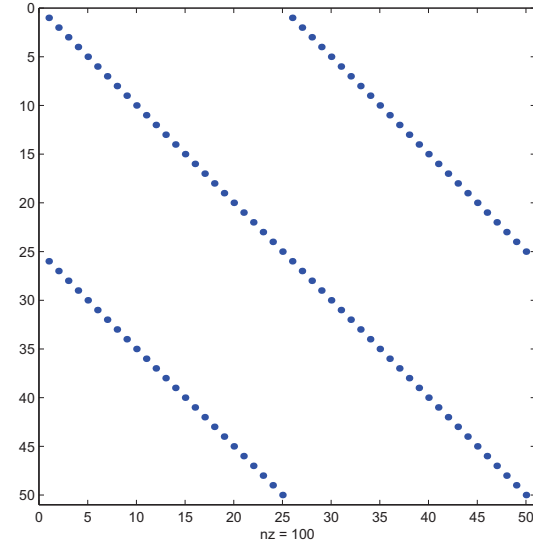


Figure 3

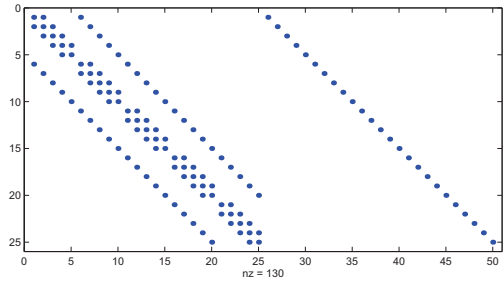


Figure 4

The Newton Interior-Point method stops when the outer residual  $\mathbf{H}(\mathbf{v}^{(k)})$  satisfies the rule

$$\|\mathbf{H}(\mathbf{v}^{(k)})\| \leq 10^{-8}$$

or when

$$\frac{|\text{gap}|}{1 + |\text{gap}|} \leq 10^{-8}$$

where “gap” is the difference between the primal function  $f(\mathbf{x})$  and the dual function (see [3]).

The inner Hestenes solver stops if the inner residual  $\mathbf{r}^{(k)}$  satisfies the following rule

$$\|\mathbf{r}^{(k)}\| \leq \max(5 \cdot 10^{-8}, \delta_k \|\mathbf{H}(\mathbf{v}^{(k)})\|)$$



Table 1: features of the test problems

Name of the problem	Problem	$N_h$	$\alpha$	$M$	$K$	$u_1$	$u_2$	$\psi(x_1, x_2)$
1-0.005-59	1	60	0.005					
1-0.005-119	1	120	0.005					
1-0.005-179	1	180	0.005					
1-0-59	1	60	0					
1-0-119	1	120	0					
1-0-179	1	180	0					
2-1-49	2	50		1	0.8	1.7	2	7.1
2-1-99	2	100		1	0.8	1.7	2	7.1
2-1-199	2	200		1	0.8	1.7	2	7.1
2-0-49	2	50		0	1	2	6	4.8
2-0-99	2	100		0	1	2	6	4.8
2-0-199	2	200		0	1	2	6	4.8

or if a maximum number of iterations is reached; in the experiments, the maximum number is fixed equal to 15. Here  $\delta_k$  is a suitable parameter that guarantees the convergence of the Inexact IP method (see [6]).

At each Hestenes iteration, the Cholesky factorization of  $A + \chi BB^t$  is obtained by a Fortran package of Ng and Peyton ([13]). For the parameter  $\chi$ , see formula (10).

In the Table 2, results on the iteration of Newton Inexact Interior-Point method are reported. “IP It.” denotes the outer iteration while “It. Hestenes” denotes the total amount of Hestenes iterations that must be performed, “time” is the elapsed time expressed in seconds and “Minimum” is the minimum value of the objective function. In figure 5, we show the behaviour of the inner and outer residuals at each iteration of the IP scheme.

Table 2: numerical results

Test-problem	$n$	$neq$	IP It.	It. Hestenes	time (s.)	Minimum
1-0.005-59	3717	3618	21	21	1.85	0.27897283
1-0.005-119	14637	14518	31	31	19.04	0.25908196
1-0.005-179	32757	32578	37	37	78.39	0.25305434
1-0-59	3717	3618	22	22	1.88	0.17710729
1-0-119	14637	14518	31	31	19.04	0.15741542
1-0-179	32757	32578	47	47	101.22	0.15128355
2-1-49	4802	2401	21	23	1.66	-6.4857812
2-1-99	19602	9801	28	29	14.52	-6.5764273
2-1-199	79202	39601	48	49	150.49	-6.6200923
2-0-49	4802	2401	33	34	2.60	-18.4825400
2-0-99	19602	9801	45	46	23.03	-18.7361483
2-0-199	79202	39601	54	97	180.18	-18.8633116

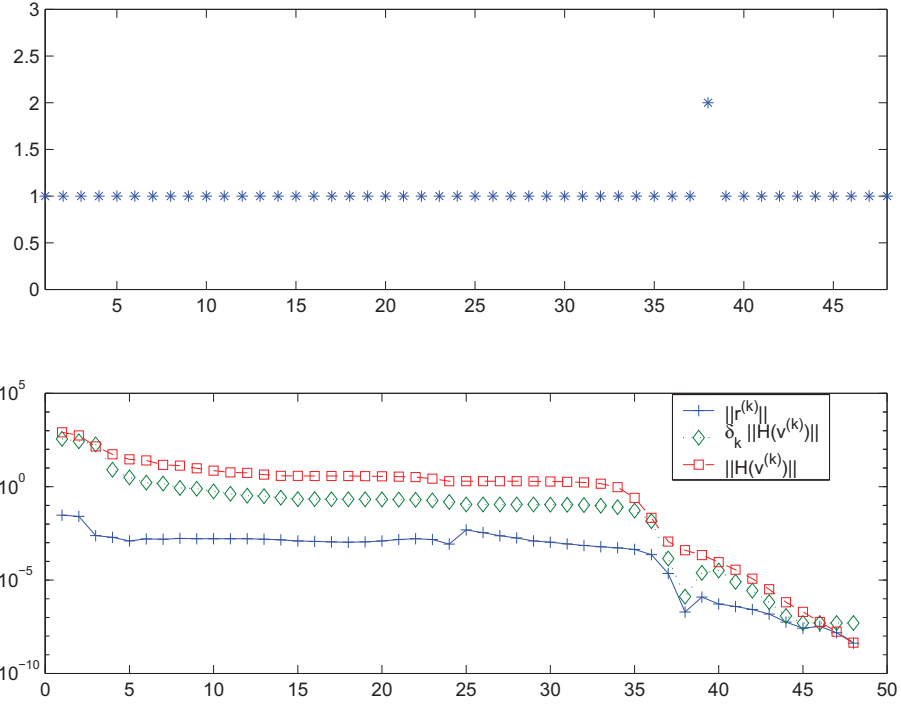


Figure 5: inner iterations per outer IP iterations for 2-1-199

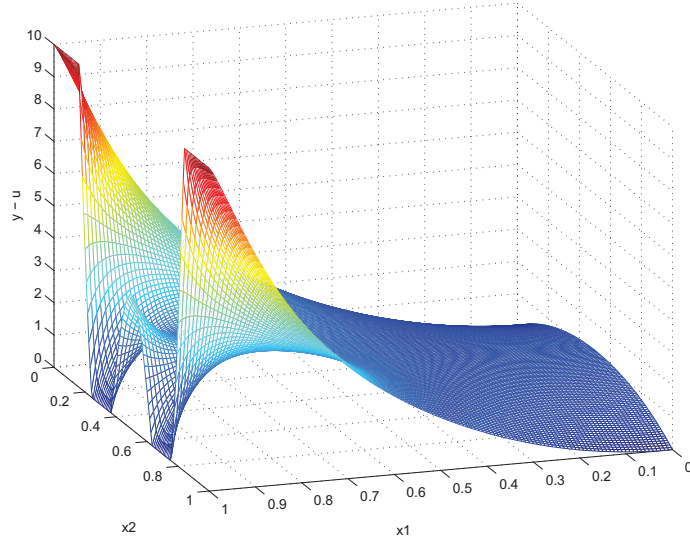


Figure 6: optimal state and control for test problem 1-0.005-119

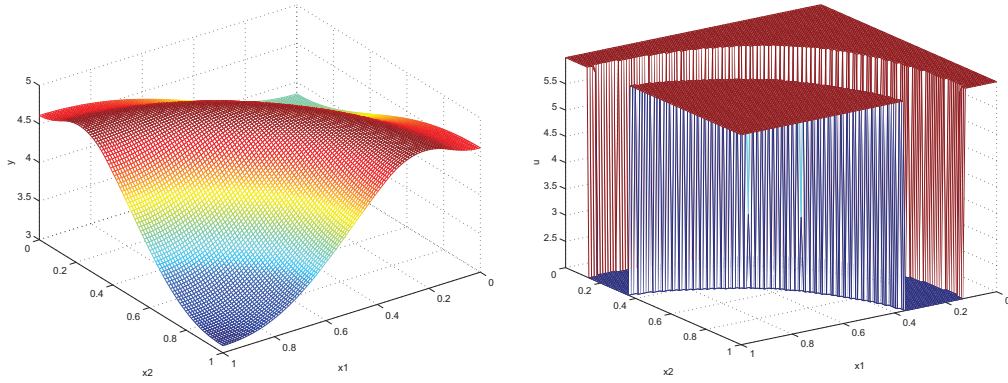


Figure 7: optimal state and control for test problem 2-0-99

In the Table 3, we report a comparison in terms of outer iterations and computer time between Newton Interior-Point method with iterative Hestenes solver and Newton Interior-Point method with a direct solver (MA27, Harwell Subroutine Library).

Figure 6 shows the optimal control and state of the boundary control problem 1-0.005-119, while in the Figure 7 the optimal state (left) and control (right) of the distributed control problem 2-0-99 are displayed. As we notice, a bang-bang control occurs in this case.

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Table 3: comparison direct–iterative inner solvers

Test-problem	IP It.	It. Hestenes	time (s.)	IP It. (MA27)	time (s.)
1-0.005-59	21	21	1.85	26	21.25
1-0.005-119	31	31	19.04	31	315.80
1-0-59	22	22	1.88	27	11.94
1-0-119	31	31	19.04	35	175.01
2-1-49	21	23	1.66	25	6.04
2-1-99	28	29	14.52	25	71.30
2-1-199	48	49	150.49	26	1008.7
2-0-49	33	34	2.60	31	176.47

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